DTU Library

Simulation tools for detector and instrument design

Kanaki, Kalliopi; Kittelmann, Thomas; Cai, Xiao Xiao; Klinkby, Esben Bryndt; Knudsen, Erik B.; Willendrup, Peter Kjær; Hall-Wilton, Richard

Published in:
Physica B: Condensed Matter

Link to article, DOI:
10.1016/j.physb.2018.03.025

Publication date:
2018

Document Version
Version created as part of publication process; publisher's layout; not normally made publicly available

Citation (APA):
Kanaki, K., Kittelmann, T., Cai, X. X., Klinkby, E. B., Knudsen, E. B., Willendrup, P. K., & Hall-Wilton, R. (2018). Simulation tools for detector and instrument design. *Physica B: Condensed Matter*, *551*, 386-389. https://doi.org/10.1016/j.physb.2018.03.025

ARTICLE IN PRESS

Physica B: Condensed Matter xxx (2018) 1–4

Contents lists available at ScienceDirect

Physica B: Condensed Matter

journal homepage: www.elsevier.com/locate/physb

Simulation tools for detector and instrument design

Kalliopi Kanaki [a,*], Thomas Kittelmann [a], Xiao Xiao Cai [a,b], Esben Klinkby [b,a], Erik B. Knudsen [b], Peter Willendrup [b,a], Richard Hall-Wilton [a,c]

[a] European Spallation Source ERIC, 22-100, Lund, Sweden
[b] Technical University of Denmark, DTU, 2800 Kgs. Lyngby, Denmark
[c] Mid-Sweden University, SE-851 70 Sundsvall, Sweden

ARTICLE INFO

Keywords:
Crystals
File formats
Monte Carlo simulations
Neutron detector
Neutron scattering

ABSTRACT

The high performance requirements at the European Spallation Source have been driving the technological advances on the neutron detector front. Now more than ever is it important to optimize the design of detectors and instruments, to fully exploit the ESS source brilliance. Most of the simulation tools the neutron scattering community has at their disposal target the instrument optimization until the sample position, with little focus on detectors. The ESS Detector Group has extended the capabilities of existing detector simulation tools to bridge this gap. An extensive software framework has been developed, enabling efficient and collaborative developments of required simulations and analyses – based on the use of the `Geant4` Monte Carlo toolkit, but with extended physics capabilities where relevant (like for Bragg diffraction of thermal neutrons in crystals). Furthermore, the `MCPL` (Monte Carlo Particle Lists) particle data exchange file format, currently supported for the primary Monte Carlo tools of the community (`McStas`, `Geant4` and `MCNP`), facilitates the integration of detector simulations with existing simulations of instruments using these software packages. These means offer a powerful set of tools to tailor the detector and instrument design to the instrument application.

1. Introduction

The neutron scattering community has been investing a large effort in developing new detector technologies that can tackle the needs of the upcoming European Spallation Source (ESS) [1]. The detector designs are diverse and target different sets of requirements [2,3], e.g.high spatial resolution [4,5], high rate capability [5,6], large area coverage [7] or combinations thereof. Additionally, as instrument performance is typically defined by the signal to background ratio [8], the ability to predict and improve instrument backgrounds will enhance the capability of future instruments. To facilitate and accelerate the design process, the use of `Geant4` [9–11] has been adopted. It is a powerful Monte Carlo simulation toolkit for the description of particle passage through matter, used by several scientific communities since decades. Specifically it provides step-based particle simulations in arbitrarily complex geometrical layouts, and with physics modeling capabilities extending beyond thermal neutrons to include also other particle types and a wide range of electromagnetic and hadronic processes – features all essential for any simulation of detector performance.

In recent years the capabilities of `Geant4` have been extended to include an increasing number of neutron-related phenomena at lower energies. The ESS Detector Group continues this effort by creating easily integrable tools, modeling Bragg and inelastic processes in crystalline materials. This way, it is becoming possible to expand the relevant functionality of `Geant4` and other software packages utilized by the neutron scattering community. A selection of these tools is presented in this article with focus on their functionality and not their technical implementation. The intention of these tool-sets is two-fold: firstly to enhance the capability and accuracy of the simulations; secondly to lower the entry barrier to utilization of the simulation codes and ensure their correct usage with modern code management and validation of the code and standard results.

2. The `NCrystal` project

A large fraction of the instrument components consists of crystalline materials, which makes it crucial for simulations to correctly model interactions of thermal neutrons in such materials. One of the first

* Corresponding author.
E-mail address: Kalliopi.Kanaki@esss.se (K. Kanaki).

https://doi.org/10.1016/j.physb.2018.03.025
Received 8 August 2017; Received in revised form 12 March 2018; Accepted 13 March 2018
Available online XXX

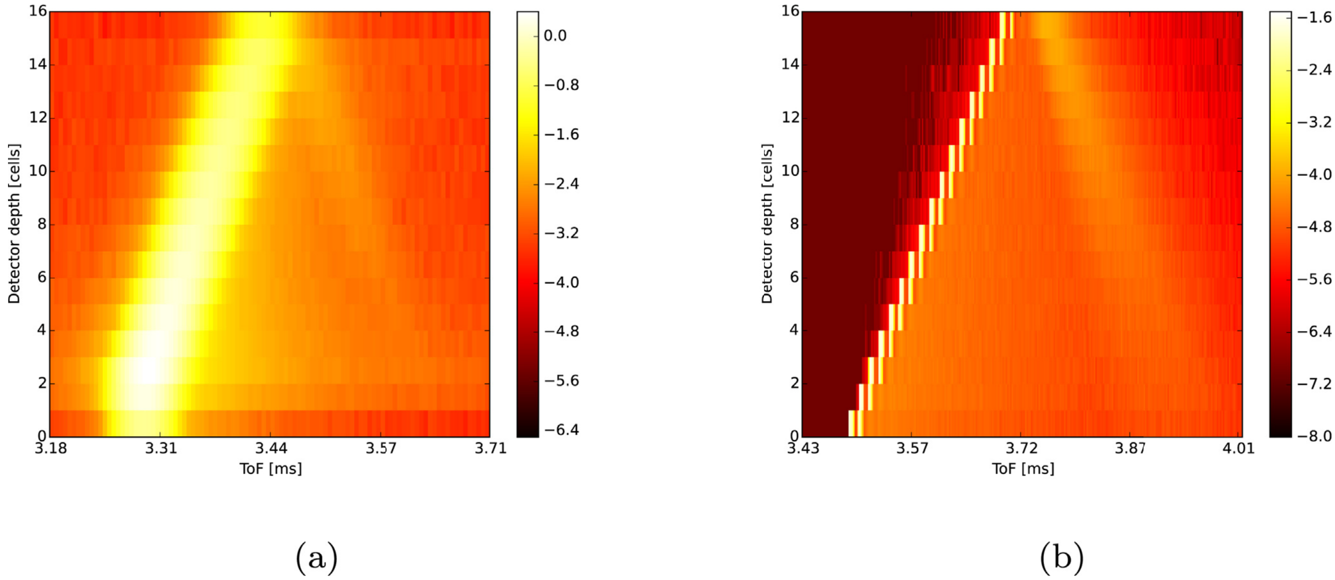

Fig. 1. Back-scattered neutrons at the rear end of the Multi-Grid detector module (a) (from Ref. [14]) can be reproduced with `Geant4` (b) (from Ref. [15]), provided the coherent scattering for the crystalline Al detector frame is enabled via `NXSG4`.

`Geant4`-extensions written for this purpose is `NXSG4` [12,13]. It provides `Geant4` with a description of Bragg scattering on a selection of powder materials. It is extensively used to study the impact of the detector material budget on the simulated detector signal. Fig. 1 demonstrates how such an effect can be reproduced by enabling the crystal properties of Aluminium in a `Geant4` simulation of the Multi-Grid detector [14,15] via `NXSG4`.

With `NXSG4` being a precursor, further advances on this front aim to expand the material functionalities, including the treatment of scattering on single-crystals, compound materials and non-Bragg processes. This effort is combined in the `NCrystal` project [16,17], which comes with appropriate extensions for integration with both `McStas` [18] and `Geant4`.

In the current state of the code, supported are Bragg scattering on powders and single crystals, as well as an improved description of inelastic and incoherent processes. A demonstration of its potential is presented in Figs. 2 and 3 for a Germanium powder and a single mosaic C_{60} crystal respectively. The code is benchmarked against experimental data for a popular list of materials, both single element (e.g. Al, Cu, Ge, Si, Be, V, Pb, C) and compound (e.g. CuO, MgO, Al_2O_3, SiO_2). Such a validation example is shown in Fig. 4 for the modeling of neutron interactions in a Cu powder.

In summary, `NCrystal` offers accurate yet efficient descriptions of neutron-crystal interactions, arguably unprecedented in a general-purpose, open source library, and is expected to play a crucial role in advancing the simulations of detector performance and instrument components, such as filters, monochromators and crystalline samples. It is available for standalone usage as well as from within both `McStas` and `Geant4`. When used in combination with the latter it enables realistic simulations with thermal neutrons in crystals, automatically including advanced features like multiple scattering in arbitrarily complex geometries.

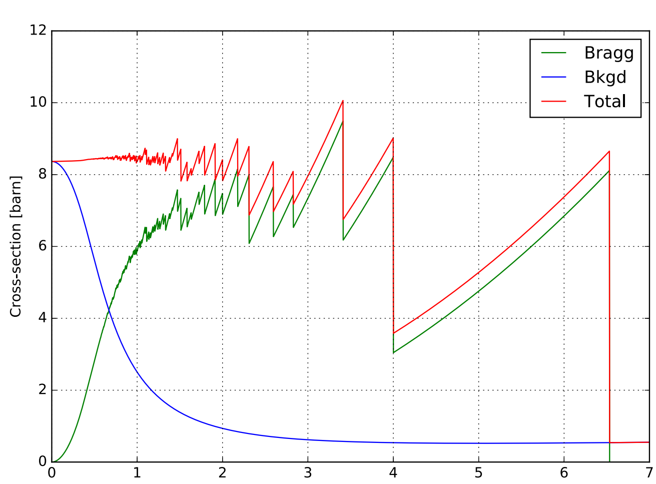

Fig. 2. Total neutron cross sections for Germanium powder as a function of neutron wavelength, overlaid with the Bragg and background contributions, provided by `NCrystal`.

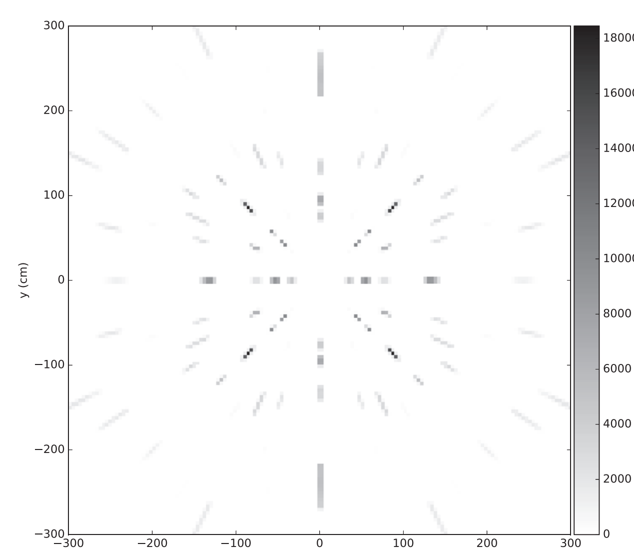

Fig. 3. Bragg diffraction pattern from a single buckminsterfullerene (C_{60}) structure, as simulated by `NCrystal`. The pattern is derived with a fixed-orientation white neutron beam hitting the crystal. Only Bragg scattering is enabled, while multiple scattering is ignored. The generated Bragg pattern shows the crystal reciprocal lattice, which is directly comparable with those obtained in neutron and X-ray measurements in a similar geometry setup.

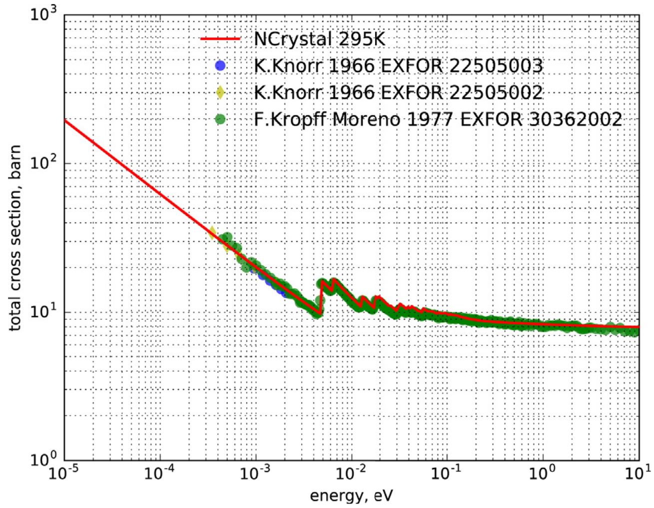

Fig. 4. Cu total cross section vs. neutron energy as predicted by `NCrystal` (red). The experimentally determined points are taken from the IAEA EXFOR database [19,20]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

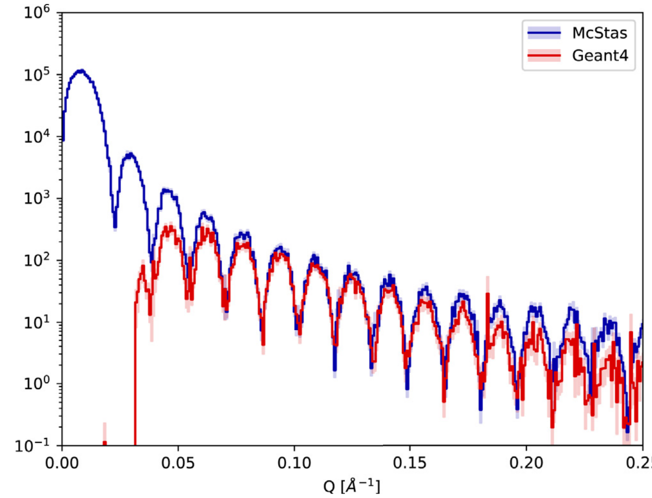

Fig. 5. Raw Q distribution for a subset of the detectors of the instrument (from Ref. [21]). The `McStas` post-sample output appears in blue, while the distribution calculated from the simulated measurements in `Geant4` appears in red. The difference is due to the physical gap of the detector coverage for angles below 0.2°. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

3. The `MCPL` file format

Motivated by the need for simulation packages to efficiently exchange particle data, the ESS Detector Group developed the Monte Carlo Particle List (`MCPL`) file format [21]. It is a well-defined, binary format containing full particle state information. Interfaces are available for `Geant4`, `McStas` 2.4.1, `McXtrace` 1.4 [22], `MCNP5` [23], `MCNP6` and `MCNPX`, so that the communication between these packages is facilitated through a single standardized format. `MCPL` comes with C/C++/Python bindings that allow easy integration with software packages. It also constitutes a convenient way for storage of particle state information even for users of just a single software application. The stand-alone code can be downloaded from its GitHub repository [24], is open source and released under very liberal license conditions. The power of the `MCPL` format lies in its flexibility and efficient implementation but also in the utilities it ships with. Easy histogram visualization, file merging, filtering and modification are available via simple terminal commands [25]. The `MCPL` format allows the most appropriate or familiar simulation code to be used by the user for the application foreseen.

As a show case for the `MCPL` use, the interfacing of a `McStas` instrument simulation to a `Geant4` detector simulation is presented here. As a part of the detector and instrument optimization processes, it is beneficial to use customized input for the detector simulation, e.g.a realistic distribution of neutrons scattered from a typical sample for the particular application. Such a scenario is shown in Fig. 5. Neutrons are simulated in a Small Angle Neutron Scattering instrument in `McStas` until after their scattering on 200 Å radius spheres. These neutrons are then saved with all their properties in the `MCPL` format and used as input to a `Geant4` simulation, which contains a detailed detector model. This way, the user is able to look at the interesting scientific quantities both at the sample and after the detection or any other stage of the simulation. In this particular example, Fig. 5 depicts the Q intensity that contains instrument and sample effects in blue, while in red appears the result of the `Geant4` detector simulation, which additionally convolves the detector effects.

4. The ESS simulation framework

It is customary for large scientific communities to create software frameworks, which provide support and utilities to all community members. These should incorporate modern software coding tools such as a versioned repository, documentation, issue tracking and validation [26–29]. Such a simulation framework [30] has been developed by the ESS Detector Group and is used at the moment within ESS and by in-kind collaborators in Europe. It facilitates a quick setup of simulation and analysis of new projects, reducing thus the overhead required to start a new detector simulation. Users can benefit from centralized support and utilities that are seamlessly integrated. To mention just a few of the latter, the framework ships with a user-friendly, dynamic build system, a flexible Python interface for combining geometries and particle generators, a dedicated 3D viewer based on `OpenSceneGraph` [31] that allows visualization and quick geometry debugging (see Fig. 6), a customized binary file format (`GRIFF`) [30] for efficient storage of simulation output and accompanying meta-data, and finally NumPy-compatible histogram classes to assist the user with the analysis of the results. In addition to these utilities, all the aforementioned libraries

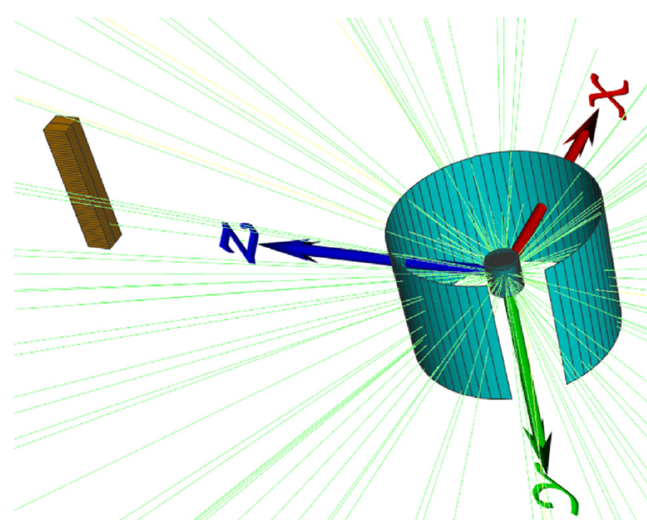

Fig. 6. Geometry and particle gun visualization with the ESS simulation framework viewer. The neutrons are generated at the centre of the coordinate system and are emitted isotropically towards the Multi-Grid detector modules (in orange). The turquoise volumes represent Aluminium components of the sample environment and the entrance window. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

(NXSG4, NCrystal, MCPL) are already incorporated and ready to use.

5. Outlook

The instrument and detector requirements at ESS place high demands on the respective simulation tools to tackle the ambitious design challenges. With the advances outlined in this article, it is now possible to accurately model an ever larger fraction of instrument and detector components. Focus has been given to the inclusion of relevant physics processes, as well as the communication between the simulation tools of the community, facilitating the tailoring of the detector designs to the scientific application. This allows the most appropriate simulation program to be used for the particular task in-hand.

Acknowledgments

This work was supported in part by the EU Horizon 2020 framework, BrightnESS project 676548.

References

[1] S. Peggs, et al., ESS Technical Design Report, ESS 2013-001 2013, http://esss.se/scientific-technical-documentation.
[2] O. Kirstein, et al., Neutron position sensitive detectors for the ESS, in: Proceedings of Science (Vertex), 2014, p. 029.
[3] BrightnESS website, https://brightness.esss.se/.
[4] D. Pfeiffer, F. Resnati, J. Birch, M. Etxegarai, R. Hall-Wilton, C. Höglund, L. Hultman, I. Llamas-Jansa, E. Oliveri, E. Oksanen, L. Robinson, L. Ropelewski, S. Schmidt, C. Streli, P. Thuiner, First measurements with new high-resolution gadolinium-GEM neutron detector, J. Instrum. 11 (2016) P05011, https://doi.org/10.1088/1748-0221/11/05/P05011.
[5] F. Piscitelli, F. Messi, M. Anastasopoulos, T. Bryś, F. Chicken, E. Dian, J. Fuzi, C. Höglund, G. Kiss, J. Orban, P. Pazmandi, L. Robinson, L. Rosta, S. Schmidt, D. Varga, d T. Zsiros, R. Hall-Wilton, The Multi-Blade Boron-10-based neutron detector for high intensity neutron reflectometry at ESS, J. Instrum. 12 (03) (2017) P03013, https://doi.org/10.1088/1748-0221/12/03/P03013.
[6] G. Albani, E. Perelli Cippo, G. Croci, A. Muraro, E. Schooneveld, A. Scherillo, R. Hall-Wilton, K. Kanaki, C. Höglund, L. Hultman, J. Birch, G. Claps, F. Murtas, M. Rebai, M. Tardocchi, G. Gorini, Evolution in boron-based GEM detectors for diffraction measurements: from planar to 3D converter, Meas. Sci. Technol. 27 (11) (2016) 115902, https://doi.org/10.1088/0957-0233/27/11/115902.
[7] M. Anastasopoulos, R. Bebb, K. Berry, J. Birch, T. Bryś, J.-C. Buffet, J.-F. Clergeau, P.P. Deen, G. Ehlers, P. van Esch, S.M. Everett, B. Guerard, R. Hall-Wilton, K. Herwig, L. Hultman, C. Höglund, I. Iruretagoiena, F. Issa, J. Jensen, A. Khaplanov, O. Kirstein, I. Lopez Higuera, F. Piscitelli, L. Robinson, S. Schmidt, I. Stefanescu, Multi-grid detector for neutron spectroscopy: results obtained on time-of-flight spectrometer CNCS, J. Instrum. 12 (04) (2017) P04030, https://doi.org/10.1088/1748-0221/12/04/P04030.
[8] N. Cherkashyna, et al., Overcoming high energy backgrounds at pulsed spallation sources, in: Proceedings of ICANS XXI Conference, 2014. arXiv:1501.02364.
[9] S. Agostinelli, et al., Geant4 —- a simulation toolkit, Nucl. Instrum. Meth. Phys. Res. 506 (2003) 250–303, https://doi.org/10.1016/S0168-9002(03)01368-8.
[10] J. Allison, et al., Geant4 developments and applications, IEEE Trans. Nucl. Sci. 53 (2006) 270–278, https://doi.org/10.1109/TNS.2006.869826.
[11] J. Allison, et al., Recent developments in Geant4, Nucl. Instrum. Meth. Phys. Res. 835 (2016) 186–225, https://doi.org/10.1016/j.nima.2016.06.125.
[12] T. Kittelmann, M. Boin, Polycrystalline neutron scattering for Geant4: NXSG4, Comput. Phys. Commun. 189 (2015) 114–118, https://doi.org/10.1016/j.cpc.2014.11.009.
[13] NXSG4 Website, 2014, http://nxsg4.web.cern.ch/nxsg4/.
[14] J. Birch, J.-C. Buffet, J.-F. Clergeau, J. Correa, P. van Esch, M. Ferraton, B. Guerard, J. Halbwachs, R. Hall-Wilton, L. Hultman, C. Höglund, A. Khaplanov, M. Koza, F. Piscitelli, M. Zbiri, In-beam test of the Boron-10 Multi-Grid neutron detector at the IN6 time-of-flight spectrometer at the ILL, J. Phys. Conf. 528 (2014) 012040, https://doi.org/10.1088/1742-6596/528/1/012040.
[15] E. Dian, K. Kanaki, R. Hall-Wilton, A. Khaplanov, T. Kittelmann, Shielding optimization study for ^{10}B-based large area neutron detectors with detailed Geant4 model, in: Proceedings of NSS-MIC IEEE Conference, Strasbourg, 2016. paper N28–18.
[16] X.X. Cai, T. Kittelmann, NCrystal GitHub Repository, 2018, https://mctools.github.io/ncrystal/.
[17] X.X. Cai, T. Kittelmann, NCrystal Release 0.9.7, 2018, https://zenodo.org/record/1189574.
[18] McStas - A neutron ray-trace simulation package, http://mcstas.org/.
[19] N. Otuka, et al., Towards a more complete and accurate experimental nuclear reaction data library (EXFOR): international collaboration between nuclear reaction data centres (NRDC), Nucl. Data Sheets 120 (2014) 272–276, https://doi.org/10.1016/j.nds.2014.07.065.
[20] Experimental Nuclear Reaction Data (EXFOR), https://www-nds.iaea.org/exfor/exfor.htm.
[21] T. Kittelmann, E. Klinkby, E.B. Knudsen, P. Willendrup, X.X. Cai, K. Kanaki, Monte Carlo particle lists: MCPL, Comput. Phys. Commun. 218 (2017) 17–42, https://doi.org/10.1016/j.cpc.2017.04.012.
[22] McXtrace - An X-ray ray-trace simulation package, http://www.mcxtrace.org/.
[23] A General Monte Carlo N-Particle (MCNP) Transport Code, https://mcnp.lanl.gov/.
[24] T. Kittelmann, et al., MCPL Documentation and GitHub Repository, 2018, https://mctools.github.io/mcpl/.
[25] T. Kittelmann, MCPL 1.2.0 with Native python Support, 2017, https://doi.org/10.5281/zenodo.822625.
[26] GitHub, Inc., https://github.com/.
[27] Atlassian Confluence for document collaboration, https://www.atlassian.com/software/confluence.
[28] Atlassian Jira Software for project and issue tracking, https://www.atlassian.com/software/jira.
[29] Atlassian Bitbucket for Git and Mercurial code management, https://www.atlassian.com/software/bitbucket.
[30] T. Kittelmann, I. Stefanescu, K. Kanaki, M. Boin, R. Hall-Wilton, K. Zeitelhack, Geant4 based simulations for novel neutron detector developmen, J. Phys. Conf. 513 (2014) 022017, https://doi.org/10.1088/1742-6596/513/2/022017.
[31] The OpenSceneGraph Project Website, http://www.openscenegraph.org/.